



chain nodes :
 13 15 22 35 40 41 43 44
 ring nodes :
 1 2 3 4 5 6 7 8 9 10 16 17 18 19 20 21 23 24 25 26 27 28 29 30 31 32
 33 34
 chain bonds :
 1-40 4-41 13-15 13-20 22-27 33-35 41-43 43-44
 ring bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19 19-20
 20-21 23-24 23-28 24-25 25-26 26-27 27-28 29-30 29-34 30-31 31-32 32-33 33-34
 exact/norm bonds :
 1-40 4-41 13-15 22-27 33-35 41-43 43-44
 exact bonds :
 13-20
 normalized bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19 19-20
 20-21 23-24 23-28 24-25 25-26 26-27 27-28 29-30 29-34 30-31 31-32 32-33 33-34

 G1:C,N
 G2:O,S,N
 G3:[*1], [*2], [*3]
 G4:C,S,N
 Match level :
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 13:CLASS
 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS 23:Atom 24:Atom
 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom
 35:CLASS 40:CLASS 41:CLASS 43:CLASS 44:Atom

